Interstitial defects stability in FeCr alloys vs Cr concentration

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Abstract

Finding adequate materials to withstand the demanding conditions in the future fusion and fission reactors is a real challenge in the development of these technologies. Structural materials need to sustain high irradiation doses and temperatures that will change the microstructure over time. A better understanding of the changes produced by the irradiation will allow for a better choice of materials, ensuring a safer and reliable future power plants. High-Cr ferritic/martensitic steels head the list of structural materials due to their high resistance to swelling and corrosion. However, it is well known that these alloys present a problem of embrittlement, which could be caused by the presence of defects created by irradiation as these defects act as obstacles for dislocation motion. Therefore, the mechanical response of these materials will depend on the type of defects created during irradiation. In this work, we address a study of the effect Cr concentration has on single interstitial defect formation energies in FeCr alloys.

Methodology

Molecular static calculations with the interatomic empirical potential specially developed by Alfredo Caro et al. for the study of FeCr alloys based in the concentration dependent model[1]. Size cells: 2000 atoms + 1 interstitial atom which could be Fe or Cr. Code: MDCASK.

Results and Discussion

Cr concentration effect:

- Calculations for concentrations of Cr in the range 1 – 17 %
- 2000 calculations for each concentration varying the relative positions of the Cr atoms randomly
- Initial interstitial atoms considered are FeFe and FeCr in three configurations: <100>, <110> and <111>
- The final configuration after optimization has been analyzed to check if it has the same direction and character (FeFe, FeCr) as the original one
- A program was developed to verify the optimised configuration

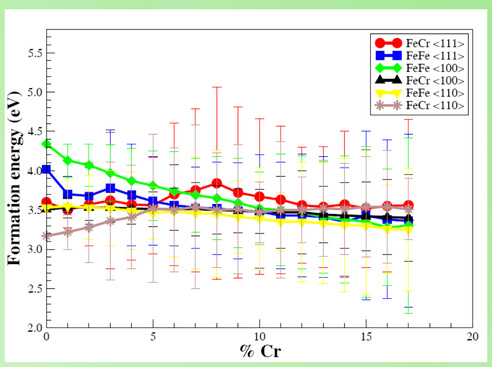


Figure 1. Average formation energy (over 2000 cases) of the different configurations as a function of Cr concentration. All cases included, independently of the final geometry reached after optimization.

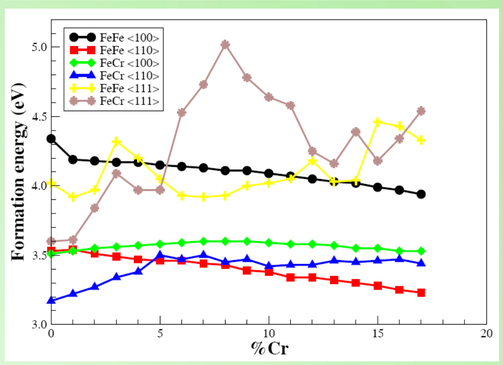


Figure 2. Average formation energy of the different configurations as a function of Cr concentration. Only those cases where the initial and final configurations are the same are considered.

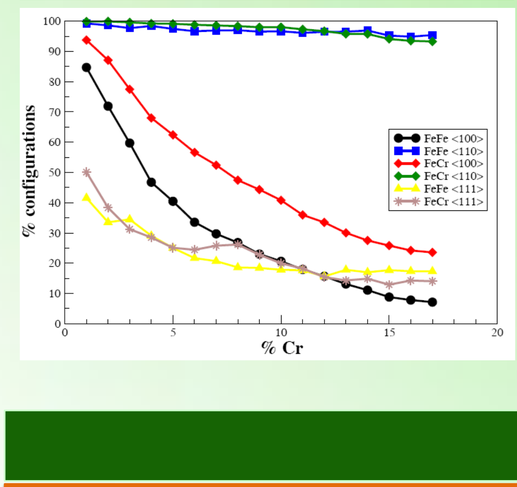
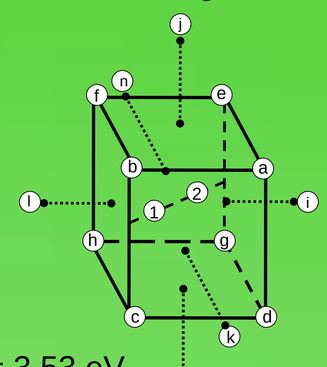


Figure 3. Percentage of configurations that do not change geometry or character used in the calculation of average formation energy of figure 2.

Local Cr distribution effect:

- Calculation of formation energies of FeFe <110> and FeCr <110> when changing the local environment: one Cr atom at different first and second nearest neighbors.

Cr_{subst}	E_f	D_{1-2}	$D_{Cr\ subst-2}$
a, e	3.47	0.740	0.721
c, h	3,47	0.740	1.302
d, g	3.42	0.737	0.927
b, f	3.42	0.737	0.927
i, j	3.49	0.738	0.765
l, m	3.49	0.739	1.328
k, n	3.52	0.733	1.040

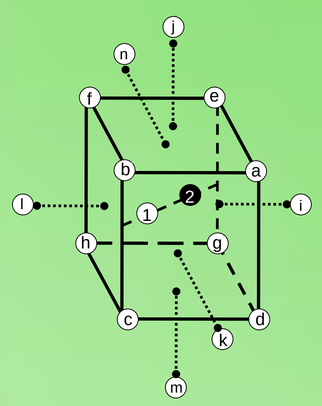


E_f = 3.53 eV
D_{1-2} = 0.736
D_{2-a} = **D_{2-e}** = 0.763
D_{2-d} = **D_{2-g}** = 0.923
D_{2-b} = **D_{2-f}** = 0.923
D_{2-c} = **D_{2-h}** = 1.318
D_{2-i} = **D_{2-j}** = 0.817
D_{2-k} = **D_{2-n}** = 1.054
D_{2-l} = **D_{2-m}** = 1.323

○ Fe atoms ● Cr atoms

D_{1-2} = distance between interstitial atoms

$D_{Cr\ subst-2}$ = distance between the interstitial atom 2 and the Cr atom at the substitution position, i.e. a, b, c, d, e, f, g, h, i, j, k, l, m, or n



Cr_{subst}	E_f	D_{1-2}	$D_{Cr\ subst-2}$
a, e	3.85	0.709	0.799
c, h	3,16	0.714	1.301
d, g	3.29	0.712	0.958
b, f	3.29	0.712	0.958
i, j	3.44	0.711	0.862
l, m	3.18	0.714	1.338
k, n	3.32	0.711	1.029

E_f = 3.15 eV
D_{1-2} = 0.7132
D_{2-a} = **D_{2-e}** = 0.7289
D_{2-b} = **D_{2-f}** = 0.9111
D_{2-d} = **D_{2-g}** = 0.9537
D_{2-h} = **D_{2-c}** = 1.3182
D_{2-i} = 0.8449
D_{2-j} = 0.7742
D_{2-k} = **D_{2-n}** = 1.0468
D_{2-l} = 1.3055
D_{2-m} = 1.3545

- $E_f = E_{defect} - (E_{without\ defect} + E_{interst})$

E_f = Formation energy of the defect

E_{defect} = Energy of the cell with a defect

$E_{without\ defect}$ = Energy of the cell without a defect

$E_{interst}$ = Energy of the Fe (FeFe interstitial) or Cr (FeCr interstitial) perfect cell per atom

Conclusions

- Formation energies converge to a unique value with Cr concentration as can be seen in Figure 1, independently of the starting geometry.
- <110> configurations are the most stable comparing with <100> and <111> configurations
- It is observed a change in the stability of <110> interstitials with Cr concentration:
  - 0 – 5% Cr, FeCr is the most stable
  - 6 – 10% Cr, same stability for self and mixed interstitials
  - 11 – 17% Cr, FeFe is the most stable
- The local Cr distribution study shows that:
  - Formation energy depends strongly on Cr position for the case of FeCr <110> interstitials and weakly in the case of FeFe <110> interstitials.
  - The shorter the distance between Cr atoms, the greater the formation energy

References

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c – E. del Rio, J. M Sampedro, H. Dogo, M. J. Caturla, M. Caro, A. Caro and J. M. Perlado. J. Nucl. Mater. 408 (2011) 18-24.

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